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Partial Ferromagnetism in Semimetallic Two-Band Models

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Stimulated by the high-temperature ferromagnetism (HTF) recently found in doped hexaborides ($D_{1-x}La_xB_6$, D=Ca,Sr,Ba),[1] ferromagnetism in semimetallic systems has attracted renewed interest. Actually, these hexaborides have a semimetallic band structure as shown by the LDA calculations.[2-5] One of possible mechanisms to explain HTF may be weak ferromagnetism in doped excitonic insulator.[6-9] However, the excitonic ferromagnet accompanies two phase transitions which have not been observed in hexaborides. To explore whether electron-hole systems favor ferromagnetism, we have numerically investigated a Hubbard-like model with a semimetallic band structure in one- and infinite-dimensional systems. By performing the density-matrix-renormalization-group calculation, we construct the ground-state phase diagram specified by interaction strength and the electron density.[10] We find that the partially ferromagnetic state is realized by doping the compensated semimetal in the intermediate-coupling regime. The inter-orbital attractive force due to the Hund's-rule coupling is indispensable for the appearance of this ferromagnetism. We show that the semimetallic band structure favors ferromagnetism, which appears by the interactions in the order of the band overlap. We have also confirmed the appearance of the partially ferromagnetic state by performing the dynamical-mean-field-theory calculation. Based on these accurate calculations, we discuss the mechanism of HTF observed in the hexaborides and speculate on its relevance to other materials such as CaB_2C_2.

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